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Working Paper

Original Citation:

Biyikoglu, Türker and Leydold, Josef (2006) Largest Eigenvalues of Degree Sequences. *Research Report Series / Department of Statistics and Mathematics*, 35. Department of Statistics and Mathematics, WU Vienna University of Economics and Business, Vienna.

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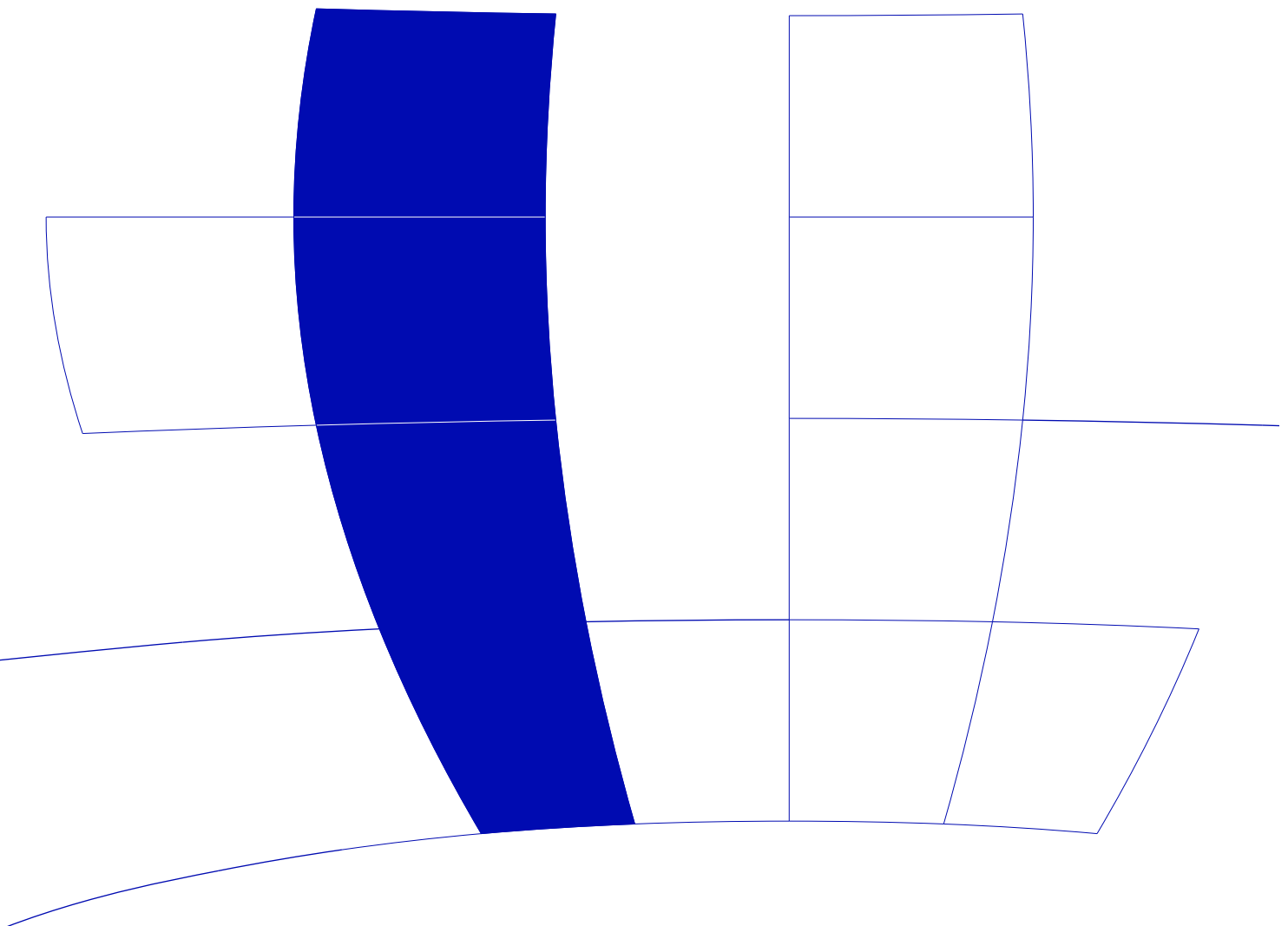


Department of Statistics and Mathematics
Wirtschaftsuniversität Wien

Research Report Series

Report 35
May 2006

<http://statmath.wu-wien.ac.at/>



Largest Eigenvalues of Degree Sequences

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Abstract

We show that amongst all trees with a given degree sequence it is a ball where the vertex degrees decrease with increasing distance from its center that maximizes the spectral radius of the graph (i.e., its adjacency matrix). The resulting Perron vector is decreasing on every path starting from the center of this ball. This result is also connected to Faber-Krahn like theorems for Dirichlet matrices on trees. The above result is extended to connected graphs with given degree sequence. Here we give a necessary condition for a graph that has greatest maximum eigenvalue. Moreover, we show that the greatest maximum eigenvalue is monotone on degree sequences with respect to majorization.

Key words: adjacency matrix, eigenvalues, eigenvectors, spectral radius, degree sequence, Perron vector, tree

1 Introduction

Let $G(V, E)$ be a simple finite undirected graph with vertex set $V(G)$ and edge set $E(G)$. $A(G)$ denotes the adjacency matrix of the graph. The spectral radius of G is the largest eigenvalue of $A(G)$. When G is connected, then $A(G)$

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¹ This paper presents research results of the Belgian Programme on Interuniversity Attraction Poles, initiated by the Belgian Federal Science Policy Office, and a grant Action de Recherche Concertée (ARC) of the Communauté Française de Belgique. The scientific responsibility rests with its authors.

is irreducible and by the Perron-Frobenius Theorem (see e.g. [7]) the largest eigenvalue $\lambda(G)$ of G is simple and there is a unique positive unit eigenvector. We refer to such an eigenvector as the *Perron vector* of G .

There exists vast literature that provides upper and lower bounds on the largest eigenvalue of G given some information about the graph, for previous results see [4]. Many recent results use maximum, minimum and average degrees, e.g., [6, 8, 15, 16]. Some new results are based on the entire degree sequence [3, 13].

The goal of this article is slightly shifted. We are interested in the geometrical properties of graphs with greatest maximum eigenvalue and the structure of their Perron vectors. In general we want to look at the following extremal eigenvalue problem.

Problem 1 *Give a characterization of all graphs in a given class \mathcal{C} that maximizes the spectral radius, i.e., find a graph G in \mathcal{C} with the greatest maximum eigenvalue $\lambda(G)$.*

We look at connected graphs with given degree sequence, in particular we are interested in tree sequences. We use a technique of rearranging graphs which has been developed in [1] for solving the problem of minimizing the first Dirichlet eigenvalue. Indeed, we will discuss the close relationship between this problem and the problem of finding trees with greatest maximum eigenvalue in Sect. 4. The results of this paper are stated in Sect. 2, the proofs are given in Sect. 3.

2 Degree Sequences and Largest Eigenvalue

Let $d(v)$ denote the degree of vertex v . We call a vertex v with $d(v) = 1$ a *pendant vertex* of the graph (and *leaf* in case of a tree). In the following n denotes the total number of vertices, i.e., $n = |V|$. A sequence $\pi = (d_0, \dots, d_{n-1})$ of nonnegative integers is called *degree sequence* if there exists a graph G with n vertices for which d_0, \dots, d_{n-1} are the degrees of its vertices. We enumerate the degrees such that $d_0 \geq d_1 \geq \dots \geq d_{n-1}$.

It is easy to check for a given sequence that it is a degree sequence. We refer the reader to Melnikov et al. [9] for relevant background. A degree sequence $\pi = (d_0, \dots, d_{n-1})$ is a degree sequence of a connected graph if and only if every $d_i > 0$ and $\sum_{i=0}^{n-1} d_i \geq 2(n-1)$, see [5]. As an immediate consequence we find that π is a tree sequence (i.e. a degree sequence of some tree) if and only if every $d_i > 0$ and $\sum_{i=0}^{n-1} d_i = 2(n-1)$.

We introduce the following class for which we can provide optimal results for the greatest maximum eigenvalue.

$$\mathcal{C}_\pi = \{G \text{ is a connected with degree sequence } \pi\}.$$

We introduce an ordering of the vertices v_0, \dots, v_{n-1} of a graph $G \in \mathcal{C}_\pi$ by means of breadth-first search. Select a vertex $v_0 \in G$ and begin with vertex v_0 in layer 0 as root; all neighbors of v_0 belong to layer 1. Now we continue by recursion to construct all other layers, i.e., all neighbors of vertices in layer i , which are not in layers i or $i-1$, build up layer $i+1$. Notice that all vertices in layer i have distance i from root v_0 . We call this distance the *height* $h(v) = \text{dist}(v, v_0)$ of a vertex v .

Notice that one can draw these layers on circles. Thus such an ordering is also called *spiral like ordering*, see [1, 10]. For the description of graphs that have greatest maximum eigenvalue we need the following notion.

Definition 2 (BFD-ordering) *Let $G(V, E)$ be a connected graph with root v_0 . Then a well-ordering \prec of the vertices is called breadth-first search ordering with decreasing degrees (BFD-ordering for short) if the following holds for all vertices $v, w \in V$:*

- (B1) $v \prec w$ implies $h(v) \leq h(w)$;
- (B2) if $v \prec w$, then $d_v \geq d_w$.

We call connected graphs that have a BFD-ordering of its vertices a BFD-graph.

Every graph has for each of its vertices v an ordering with root v that satisfies (B1). This can be found by the above breadth-first search. However, not all graphs have an ordering that satisfies (B2); consider the complete bipartite graph $K_{2,3}$.

With this concept we can give a necessity condition for graphs which have greatest maximum eigenvalue in a class \mathcal{C}_π .

Theorem 3 *Let G have greatest maximum eigenvalue in class \mathcal{C}_π . Then there exists a BFD-ordering of $V(G)$ that is consistent with its Perron vector f in such a way that $f(u) > f(v)$ implies $u \prec v$ and $d_u \geq d_v$.*

It is important to note that this condition is not sufficient in general. Let $\pi = (4, 4, 3, 3, 2, 1, 1)$, then there exist two BFD-graphs but only one has greatest maximum eigenvalue, see Fig. 1.

Remark 4 *If \mathcal{C}_π has a unique graph G that has a BFD-ordering, then G has greatest maximum eigenvalue in \mathcal{C}_π .*

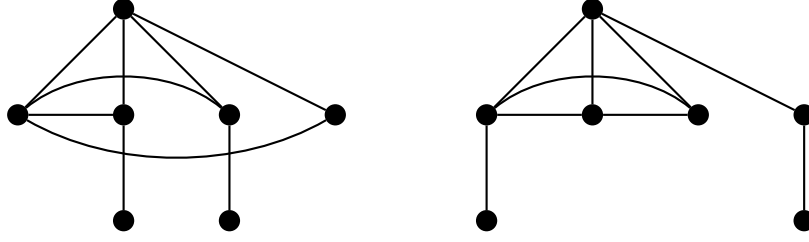


Fig. 1. Two BFD-graphs with degree sequence $\pi = (4, 4, 3, 3, 2, 1, 1)$ that satisfy the conditions of Thm. 3.

l.h.s.: $\lambda = 3.0918$, $f = (0.5291, 0.5291, 0.3823, 0.3823, 0.3423, 0.1236, 0.1236)$,

r.h.s.: $\lambda = 3.1732$, $f = (0.5068, 0.5023, 0.4643, 0.4643, 0.1773, 0.1583, 0.0559)$

Trees are of special interest. There are recent upper bounds according to degrees of a tree. For example, bounds involving the largest degree of a tree are given in [11, 12, 14]. Here we are interested in the class \mathcal{T}_π of all trees with given sequence π . Notice that this class fulfills the assumption of Remark 4.

Theorem 5 *A tree G with degree sequence π has greatest maximum eigenvalue in class \mathcal{T}_π if and only if it is a BFD-tree. G is then uniquely determined up to isomorphism. The BFD-ordering is consistent with the Perron vector f of G in such a way that $f(u) > f(v)$ implies $u \prec v$.*

Corollary 6 *For a tree with degree sequence π a sharp upper bound on the largest eigenvalue can be found by computing the corresponding BFD-tree. Obviously this can be done in $O(n)$ time if the degree sequence is sorted.*

We define a partial ordering on degree sequences as follows: for two sequences $\pi = (d_0, \dots, d_{n-1})$ and $\pi' = (d'_0, \dots, d'_{n-1})$ we write $\pi \leq \pi'$ if and only if $\sum_{i=0}^{n-1} d_i = \sum_{i=0}^{n-1} d'_i$ and $\sum_{i=0}^j d_i \leq \sum_{i=0}^j d'_i$ for all $j = 0, \dots, n-1$. Recall that the degree sequences are non-increasing. Such an ordering is also called *majorization*. The greatest maximum eigenvalues of classes \mathcal{C}_π are monotone on degree sequences with respect to ordering \leq .

Theorem 7 *Let π and π' two distinct degree sequences with $\pi \leq \pi'$. Let G and G' be graphs with greatest maximum eigenvalues in classes \mathcal{C}_π and $\mathcal{C}_{\pi'}$, resp. Then $\lambda(G) < \lambda(G')$.*

We get the following well-known result as an immediate corollary.

Corollary 8 *A tree G has greatest maximum eigenvalue in the class of all trees with n vertices and k leaves if and only if it is a star with paths of almost the same length to each of its k leaves.*

Proof. The tree sequence $\pi^* = (k, 2, \dots, 2, 1, \dots, 1)$ is maximal in the class of trees with k pendant vertices. Thus the statement immediately follows from Thms. 5 and 7. \square

3 Proof of the Theorems

We recall that $\lambda(G)$ denotes the maximum eigenvalue of G . Let $N_f(v) = \sum_{uv \in E} f(u)$. Thus the adjacency matrix $A(G)$ can be defined by $(Af)(v) = N_f(v)$. The Rayleigh quotient of the adjacency matrix $A(G)$ on vectors f on V is the fraction

$$\mathcal{R}_G(f) = \frac{\langle Af, f \rangle}{\langle f, f \rangle} = \frac{\sum_{v \in V} f(v) \sum_{uv \in E} f(u)}{\sum_{v \in V} f(v)^2} = \frac{2 \sum_{uv \in E} f(u)f(v)}{\sum_{v \in V} f(v)^2}. \quad (1)$$

Here and in the following we use a “functional” notation as this reflects the fact, that our investigations do not depend on the enumeration of the vertices. By the Rayleigh-Ritz Theorem we find the following well-known property for the spectral radius of G .

Proposition 9 ([7]) *Let \mathcal{S} denote the set of unit vectors on V . Then*

$$\lambda(G) = \max_{f \in \mathcal{S}} \mathcal{R}_G(f) = 2 \max_{f \in \mathcal{S}} \sum_{uv \in E} f(u)f(v).$$

Moreover, if $\mathcal{R}_G(f) = \lambda(G)$ for a (positive) function $f \in \mathcal{S}$, then f is an eigenvector corresponding to the largest eigenvalue $\lambda(G)$ of $A(G)$, i.e., it is a Perron vector.

Lemma 10 *Let f be the Perron vector of a connected graph G . Then $f(u) \geq f(v)$ if and only if $N_f(u) \geq N_f(v)$. Moreover, for each edge $uv \in E$ where v is a pendant vertex and u is not, $\lambda(G) = f(u)/f(v)$ and $f(u) > f(v)$.*

Proof. The first statement immediately follows from the positivity of the Perron vector and the fact that $f(v) = N_f(v)/\lambda$. For the second statement notice that the largest eigenvalue of a path with one interior vertex is $\sqrt{2}$. Thus the result follows by the well-known fact that $\lambda(H) \leq \lambda(G)$ for a connected subgraph H of G . This is an immediate consequence of (1). \square

The main techniques for proving our theorems is *rearranging* of edges with respect to the Perron vector. We need two standard types of rearrangement steps that we call *switching* and *shifting*, resp., in the following.

Lemma 11 (Switching) *Let $G(V, E)$ be a graph in class \mathcal{C}_π with $v_1u_1, v_2u_2 \in E$ and $v_1v_2, u_1u_2 \notin E$. By replacing v_1u_1 and v_2u_2 with the edges v_1v_2 and u_1u_2 we get a new graph $G'(V, E')$ with the same degree sequence π . Then for a positive vector $f \in \mathcal{S}$ we find $\mathcal{R}_{G'}(f) \geq \mathcal{R}_G(f)$, whenever $f(v_1) \geq f(u_2)$ and $f(v_2) \geq f(u_1)$.*

Moreover, if f is the Perron vector of G we find $\lambda(G') \geq \lambda(G)$, whenever $f(v_1) \geq f(u_2)$ and $f(v_2) \geq f(u_1)$. The inequality is strict if one of these two inequalities is strict.

If $G'(V, E')$ is connected it again belongs to \mathcal{C}_π .

Proof. Notice that switching does not change the degrees of the vertices. By removing and inserting edges we obtain

$$\begin{aligned}\mathcal{R}_{G'}(f) - \mathcal{R}_G(f) &= \langle A(G')f, f \rangle - \langle A(G)f, f \rangle \\ &= 2 \left(\sum_{xy \in E' \setminus E} f(x)f(y) - \sum_{uv \in E \setminus E'} f(u)f(v) \right) \\ &= 2(f(v_1)f(v_2) + f(u_1)f(u_2) - f(v_1)f(u_1) + f(v_2)f(u_2)) \\ &= 2(f(v_1) - f(u_2)) \cdot (f(v_2) - f(u_1)) \\ &\geq 0,\end{aligned}$$

and thus the first statement follows. Moreover, by Prop. 9 it follows that for the Perron vector f , $\lambda(G') \geq \mathcal{R}_{G'}(f) \geq \mathcal{R}_G(f) = \lambda(G)$. Notice that $\lambda(G') = \lambda(G)$ if and only if f is also an eigenvector corresponding to $\lambda(G')$ on G' . Then we find

$$\begin{aligned}\lambda(G)f(v_1) &= A(G)f(v_1) = f(u_1) + \sum_{wv_1 \in E \cap E'} f(w) \\ &= \lambda(G')f(v_1) = A(G')f(v_1) = f(v_2) + \sum_{wv_1 \in E \cap E'} f(w)\end{aligned}$$

and hence $f(u_1) = f(v_2)$. Analogously we derive from $A(G)f(u_1) = A(G')f(u_1)$, $f(v_1) = f(u_2)$. \square

Lemma 12 (Shifting) *Let $G(V, E)$ be a graph in class \mathcal{C}_π , and let $uv_1 \in E$ and $uv_2 \notin E$. Then by replacing edge uv_1 by the edge uv_2 we get a new graph $G'(V, E')$. We find for every positive function $f \in \mathcal{S}$, $\mathcal{R}_{G'}(f) \geq \mathcal{R}_G(f)$, whenever $f(v_2) \geq f(v_1)$. The inequality is strict if $f(v_2) > f(v_1)$.*

Proof. Analogously to the proof of Lemma 11. \square

Lemma 13 *Let f be the Perron vector of a graph G in \mathcal{C}_π . Let $vu \in E(G)$ and $vx \notin E(G)$ with $f(u) < f(x) \leq f(v)$. If $f(v) \geq f(w)$ for all neighbors w of x , then G cannot have greatest maximum eigenvalue in \mathcal{C}_π .*

Proof. Assume that such vertices exist. Construct a new graph $G'(V, E')$ with the same degree sequence π by replacing edges vu and xw by edges vx and uw . Then by Lemma 11, $\mathcal{R}_{G'}(f) > \mathcal{R}_G(f)$. It remains to show that we can choose vertex w such that G' is connected. Then $G' \in \mathcal{C}_\pi$ and hence G cannot have greatest maximum eigenvalue.

First notice that there must be a neighbor p of x that is not adjacent to u , since otherwise $N_f(x) = \sum_{wx \in E} f(w) \leq \sum_{yu \in E} f(y) = N_f(u)$ and thus by Lemma 10, $f(x) \leq f(u)$, a contradiction to our assumptions. Furthermore, x must have at least two neighbors, since otherwise we had by Lemma 10 and

assumption $f(x) > f(u)$, $f(w) = N_f(x) > N_f(u) \geq f(v)$, a contradiction to $f(w) \leq f(v)$. Since G is connected there is a simple $P_{vx} = (v, \dots, t, x)$ from v to x . Then there are four cases:

- (1) If $vu \notin P_{vx}$ and $ut \notin E(G)$, then we set $w = t$.
- (2) Else, if $vu \notin P_{vx}$ and $ut \in E(G)$, then we set w to one of the neighbors of x that are not adjacent to u .
- (3) Else, if $vu \in P_{vx}$ and all neighbors not equal t are adjacent to u . Then t cannot be adjacent to u and we set $w = t$.
- (4) Else, $vu \in P_{vx}$ and there exists a neighbor p of x , $p \neq t$, with $up \notin E(G)$. Then we set $w = p$.

In either case G' remains connected. Thus the statement follows. \square

Proof of Theorem 3. Let $n = |V|$ and let f be the Perron vector of G . We assume that the vertices of G , $V = \{v_0, v_1, \dots, v_{k-1}, v_k, \dots, v_{n-1}\}$, are numbered such that $f(v_i) \geq f(v_j)$ if $i < j$, i.e., they are sorted with respect to $f(v)$ in non-increasing order. We define a well-ordering \prec on V by $v_i \prec v_j$ if and only if $i < j$.

Now we use a series of switchings to check that condition (B1) holds for this ordering. This is done recursively, starting at v_0 . Notice that this statement is trivial for the root vertex v_0 . Now assume that we have checked that (B1) holds for all vertices v_k , $k = 1, \dots, j-1$ and we look at vertex v_j . Let r be the least index such that v_r is adjacent to some vertex $u_r \succ v_{j-1}$. We have three cases:

- (1) If v_r is adjacent to v_j , then there is nothing to do.
- (2) Else, if v_r is adjacent to some vertex $w \succ v_j$ with $f(w) = f(v_j)$, we just exchange the positions of v_j and w in the ordering \prec of V (and update the indices of the vertices).
- (3) Else, v_r is adjacent to some vertex $u \succ v_j$ with $f(u) < f(v_j)$. Moreover, for all neighbors w of v_j , $w \succ v_r$ holds, since otherwise v_j already had been checked. Thus $f(w) \leq f(v_r)$ and G cannot have greatest maximum by Lemma 13.

Consequently, if G has greatest maximum eigenvalue, then there exists an ordering \prec with respect to f such that (B1) holds.

It remains to show that this ordering also satisfies property (B2), i.e., $f(v) \geq f(w)$ implies $d(v) \geq d(w)$. Assume there are two vertices x and y such that $f(x) \geq f(y)$ but $d(y) - d(x) = c > 0$. Then we shift the last c neighbors of y (in ordering of \prec) from y to x and get a new graph G' with the same degree sequence π . Notice that there remains at least one neighbor of y that belongs to layer $h(y)$ or layer $h(y) - 1$. Thus G' is connected. Since G has greatest maximum eigenvalue by assumption and f is a Perron vector, $f(x) = f(y)$ by

Lemma 12. However, then f is also a Perron vector of G' and thus $\lambda(G')f(x) = \sum_{v \in E} f(v) + \sum_{w \in E' \setminus E} f(w) > \sum_{v \in E} f(v) = \lambda(G)f(x)$, i.e., $f(x) > f(x)$, a contradiction. \square

Remark 14 *The layers of a graph G with greatest maximum eigenvalue are edge maximal: if $v_1u_1, v_2u_2 \in E$ and $v_1v_2, u_1u_2 \notin E$, where v_1, v_2 are in i -th layer and u_1, u_2 in $i+1$ -th layer of the BDF-ordering, then replacing edges v_1u_1 and v_2u_2 by the edges v_1v_2 and u_1u_2 results in a disconnected graph G' .*

Proof of Theorem 5. The necessity condition is an immediate corollary of Thm. 3. To show that two BDF-trees G and G' in class \mathcal{T}_π are isomorphic we use a function ϕ that maps the vertex v_i in the i -th position in the BDF-ordering of G to the vertex w_i in the i -th position in the BDF-ordering of G' . By the properties (B1) and (B2) ϕ is an isomorphism, as v_i and w_i have the same degree and the images of neighbors of v_i in the next layer are exactly the neighbors of w_i in the next layer. The latter can be seen by looking on all vertices of G in the reverse BDF-ordering. Thus the proposition follows. \square

Proof of Theorem 7. Let $\pi = (d_0, \dots, d_{n-1})$ and $\pi' = (d'_0, \dots, d'_{n-1})$ be two non-increasing degree sequences with $\pi \leq \pi'$, i.e., $\sum_{i=0}^j d_i \leq \sum_{i=0}^j d'_i$ and $\sum_{i=0}^{n-1} d_i = \sum_{i=0}^{n-1} d'_i$. Assume that $\pi \neq \pi'$. We show the proposition by shifting edges recursively. By Thm. 3 there is a BFD-graph G with degree sequence π and with Perron vector f . Moreover, the BFD-ordering is consistent with f , i.e., $f(u) > f(v)$ implies $u \prec v$.

Let $\pi_0 = \pi$, $G_0 = G$, and set $s = 0$. Let k be the least position where $d_k^{(s)} < d'_k$ and let $w_s \succ v_k$ be the first vertex (in the ordering \prec) that is adjacent to a vertex $u_s \succ v_k$ with $u_s v_k \notin E(G_s)$. Then we replace edge $u_s w_s$ by $u_s v_k$ and get a new graph $G_{s+1}(V, E_{s+1})$ with degree sequence π_{s+1} where $d_k^{(s+1)} = d_k^{(s)} + 1$ and $\pi_s \leq \pi_{s+1}$. The BFD-ordering implies $f(w_s) \leq f(v_k)$ and thus by Lemma 12, $\mathcal{R}_{G_{s+1}}(f) \geq \mathcal{R}_{G_s}(f)$. If $\pi_{s+1} = \pi'$ we are done. Otherwise, increment s and repeat the shifting step. In this way we get a sequence of degree sequences π_s and corresponding graphs G_s such that $\mathcal{R}_{G_s}(f) \geq \mathcal{R}_G(f)$ which eventually stops at $\pi_t = \pi'$. That is, we get a graph G_t in class $\mathcal{C}_{\pi'}$ with $\lambda(G) \leq \mathcal{R}_{G_t}(f) \leq \lambda(G_t)$. Analogously to the proof of Thm. 3 equality only holds G_t has not greatest maximum eigenvalue and hence $\lambda(G) < \lambda(G_t)$. \square

4 Remarks

In general, we can ask the same questions for Perron vectors of generalized graph Laplacians, i.e., symmetric matrices with non-positive off-diagonal entries, see, e.g., [2]. In this paper we showed that switching and shifting operations are compatible with respect to degree sequences and used it to find

trees or connected graphs with greatest maximum eigenvalue of the adjacency matrix (notice that its negative, $-A(G)$, is a special case of generalized graph Laplacians). In [1] these operations were applied to construct graphs with the smallest first eigenvalue of the Dirichlet matrix. This is obtained from the combinatorial Laplacian by deleting rows and columns of some vertices which are called boundary vertices (usually pendant vertices). Here the corresponding minimization problems are called *Faber-Krahn*-type theorems. We refer interested reader to [2] and the references given therein. It is a challenging task to look for other graph operations and relating graph classes with respect to extremal eigenvalues and Perron eigenvectors.

One also might ask whether one can find the smallest maximum eigenvalue in a class \mathcal{C}_π by the same procedure. It is possible to apply shifting in the proof of Thm. 3 just the “other way round”. We then would arrive at trees that are constructed by breadth-first search but with increasing vertex degrees for non-pendant vertices (such trees are called SLO*-trees in [1]). Thus we would have trees that minimize the corresponding Dirichlet eigenvalue. However, this idea does not work as we have to minimize the maximum of the Rayleigh quotient. Indeed, such a result does not hold in general. Figure 2 shows a counterexample.

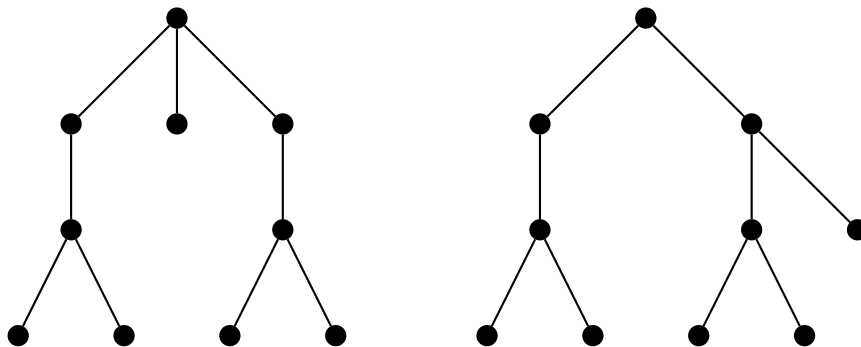


Fig. 2. Two trees with degree sequence $(2, 2, 3, 3, 3, 1, 1, 1, 1, 1)$. The tree on the l.h.s. has smallest maximum eigenvalue ($\lambda = 2.1010$) among all trees in \mathcal{C}_π . The tree on the r.h.s. has a breadth-first ordering of the vertices with increasing degree sequences (and thus has lowest first Dirichlet eigenvalue). However it does not minimize the maximum eigenvalue ($\lambda = 2.1067$)

Acknowledgment

The authors would like to thank Christian Bey to call our attention to eigenvalues of the adjacency matrix of a graph. We thank Gordon Royle and Brendan McKay for their databases of combinatorial data on graphs. This was of great help to find the two counterexamples in Figs. 1 and 2. We also thank the Institute for Bioinformatics of the University in Leipzig for the hospitality and for

providing a scientific working environment while we wrote down this paper.

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